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"Magnetic" Molecular Dynamics and Other Models for Fusion Reactor Materials

Tuesday, September 15, 2015
2:00 - 3:00pm
MSL Auditorium (TA-03 - Bldg 1698 - Room A103)

Abstract - Multiscale models for fusion reactor materials address both the initial stages of production of radiation defects, where the recently discovered power law statistics of defect production [1] provides a fundamental insight into the nature of high-energy processes occurring over the first few nanoseconds of microstructural evolution, and long-term evolution resulting in embrittlement and swelling of materials. High- resolution X-ray diffraction methods make it possible to detect swelling resulting from the accumulation of invisible radiation defects on the micron spatial scale [2], which can be explained using a hierarchy of methods involving density functional theory, atomistic simulations and statistical elasticity.

Density functional methods offer insights into the origin of phase stability of ternary magnetic alloys, where interplay between alloy disorder and magnetism determine the fine balance of stability of ferritic or austenitic, or even more complex, alloy phases [3]. Of particular interest to applications are the developments in statistical discrete treatment of dynamics of defects and dislocations [4,5], where lattice discreteness [4] and elastic interaction between the nano-scale dislocation objects [5] play unexpectedly strong roles and fundamentally influence microstructure.

The need to model magnetic materials has stimulated the development of dedicated simulation techniques, including spin-lattice dynamics [6] and magnetic cluster expansion, which generalise molecular dynamics and cluster expansion to magnetic metals and alloys. These methods extend electronic structure-based methods to time-dependent classical dynamics of atoms and magnetic moments and help explore magnetic configurations of complex alloys.

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Bio: Sergei Dudarev is Head of Materials Group at UK Atomic Energy Authority, Culham Centre for Fusion Energy, and a leader of a EURO fusion Materials subproject. Using a broad range of mathematical approaches combined with experimental observations, his group investigates physical and mechanical properties of materials in extreme radiation and temperature environments. S.L. Dudarev was born in Molodechno, Belarus, grew up in Tbilisi, Georgia, and studied theoretical and mathematical physics at Moscow Engineering Technical University (MEPhI), receiving MSc (1983) and PhD (1985) degrees in Theoretical Nuclear Physics, and DSc in 1995. In 1989 he was awarded Moscow Komsomol Prize for outstanding scientific achievements in theoretical physics, and a Royal Society USSR Research Fellowship in 1991. He worked at Oxford University, UK between 1992 and 1999, becoming a Fellow of Linacre College in 1995 and a Research Lecturer at Materials Department in 1997. He held Visiting Professorships at Hong-Kong Polytechnic University and at the University of Hong-Kong, and is now a Visiting Professor at the Department of Physics, Imperial College London, and at the Department of Materials, University of Oxford. S.L. Dudarev is an author of a book on Electron Diffraction and Microscopy published by the Oxford University Press in 2004, reprinted in paperback in 2011, and circa 200 papers in refereed academic journals on statistical theory of scattering and electron diffraction, methods of electronic structure calculations, and mathematical models for nuclear materials.

This work was funded by the RCUK Energy Programme [grant number EP/I501045], carried out within the EURO fusion Consortium and received funding from the Euratom research and training programme 2014-2018 under grant agreement number No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

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